Simulation of Ultra-Small Electronic Devices: Quantum Corrections to Classical Models

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Projects

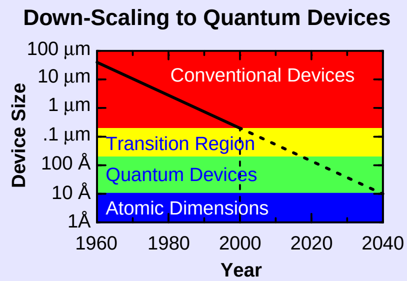
- Wigner function and transfer-matrix modeling of macroscopic quantum devices in 3-D
- Quantum corrections to classical drift-diffusion and hydrodynamic models in 3-D

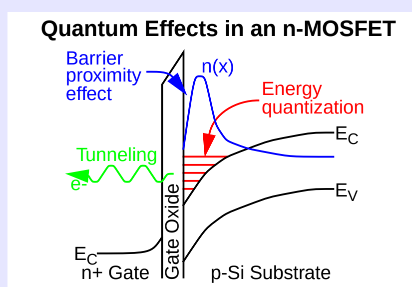
Why Model Quantum Effects in Electronics?

Parasitic quantum effects are an increasing concern in conventional electronic devices. Classical device models (such as drift-diffusion) do not describe these effects.

Modeling parasitic quantum effects would allow us to predict:

- how severe these effects will become with each future device generation
- how these effects can be suppressed
- whether and how these effects can be used to improve device operation





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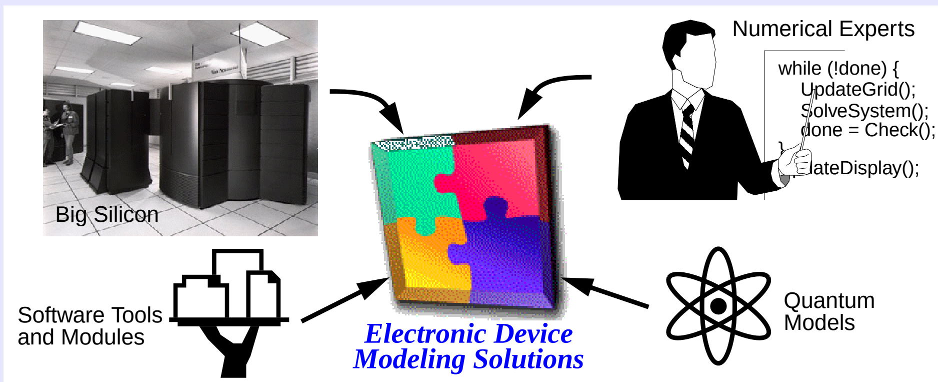
Unique NAS Resources

Approach and goals depend on available resources that can be applied:

- Supercomputing and parallel computation hardware
- Advanced numerical computation software
- Numerical computation experts
- Broad quantum device simulation experience



General Objective and Approach

General Objective: Develop 2-D and 3-D semiconductor device models including quantum effects with maximum feasible accuracy.

General Approach:

- Don’t develop or re-invent huge “vertical” application codes!
- Leverage NAS numerical software and computational hardware
- Assemble device modeling solutions from existing “generic” software modules
- Time to solution is more important than computation time
- Initially address areas of near-future interest and concern
- Compare accuracy and efficiency of various quantum models

Device Modeling: it’s not rocket science, but rocket science can give it a big boost.

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Abstract

Interest and concern is increasing about quantum effects in electronic devices as down-scaling is expected to continue through the next two decades. Technology leaders need to know how significantly parasitic quantum effects will degrade electronic device operation with each future device generation, how long these effects can be suppressed and by what means, and how quantum effects might be used to actually improve device operation. There are two main reasons why simulation tools can not yet provide this information: 1) converting new electronic device models including quantum effects into functioning simulation software is very time-consuming, and 2) the required computational resources for accurate simulations of commercially important electronic devices are immense. Both of these difficulties are addressed by this project, the goal of which is the rapid and accurate investigation of quantum effects in near-future electronic devices.

This project addresses the first issue by utilizing advanced NAS software modules and emerging third-party numerical computation tools to rapidly implement and investigate new electronic device models including quantum effects. The second issue is also addressed by the availability of highly capable parallel computation systems at NAS. Specific projects planned for this work include the investigation of quantum effects in 1-D structures using an existing quantum device simulation tool, and the rapid implementation of quantum corrections in 1-D, 2-D and 3-D to the classical drift-diffusion, hydrodynamic, and BTE models of electron transport. The test device for most of this work will be the MOSFET, in which quantum effects are the highest concern, due to its dominance in electronics and to the wide range of quantum effects which are increasingly significant in this device.

Quantum Device Simulation: Motivation

Investigate electronic systems where quantum effects are dominant:

- Gain experience in how quantum effects manifest themselves, for application to quantum corrections studies
- Knowledge of quantum models for derivation of quantum corrections
- “Map out” entire spectrum between classical and quantum realms
- Analyze capabilities of proposed/demonstrated quantum devices
- Eventually, electronics will go quantum or go nowhere - quantum simulation allows us to probe this domain before this ultimatum, and before experimental evidence is available (or at least feasible).

Progression of Electronic Devices from Classical to Quantum

Device ⇨	MOSFET BJT	MODFET HET QWLD	RTD RTT	QUIT SQUID	Quantum Dot, SET	Quantum Computer
Classical Effects	Dominant	Dominant	Significant	Parasitic	Parasitic, Negligible	Computation-killer
Quantum Effects	Parasitic	Useful	Significant	Dominant	Dominant	Exclusive

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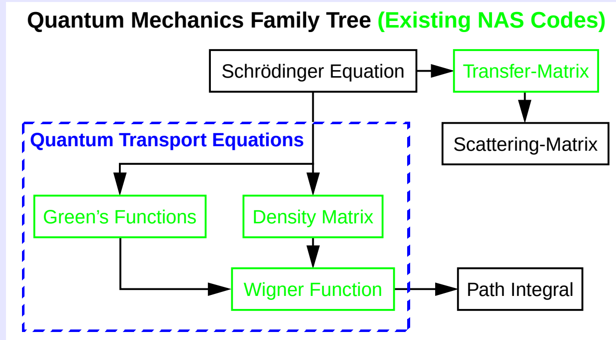
Quantum Device Simulation: Approach

Several key 1-D quantum device modeling codes exist at NAS.

Computational accuracy and efficiency will be compared.

Best formulations will be scaled to 2-D and 3-D.



This project focuses on:

- Wigner function method (quantum analogue of BTE)
  - ➩ Transient simulations, scattering, ohmic BCs
- Transfer-matrix method (standard quantum device model)
  - ➩ Computational efficiency and robustness

Quantum Device Simulation: Formulation and Challenges

Wigner Function transport equation (WFTE) in 1-D:

$$\frac{\partial f_w}{\partial t} = -\underbrace{\frac{\hbar k}{m}\frac{\partial f_w}{\partial x}}_{\text{diffusion}} - \underbrace{\frac{1}{\hbar}\int\frac{dk'}{2\pi}V(x,k-k')f_w(x,k')}_{\text{drift}} + \underbrace{\left[\frac{\partial f_w}{\partial t}\right]_{\text{coll}}}_{\text{scatering}}$$

Poisson equation in 1-D:

$$\frac{\partial}{\partial x}\left[\varepsilon(x)\frac{\partial}{\partial x}u(x)\right] = q\rho(x) = q^2[C(x)-c(x)], \quad u(x) = U(x)-\delta U(x)$$

Challenges:

- Accurate discretization of WFTE
- Computationally feasible 2-D (3-D?) simulations

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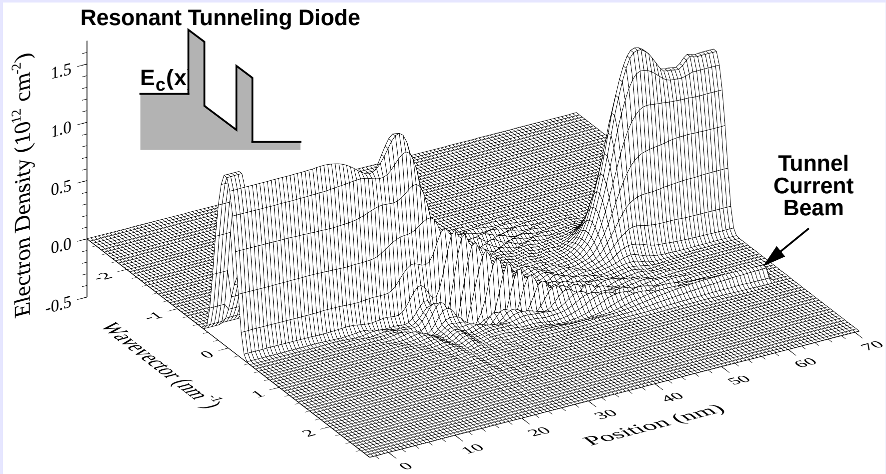
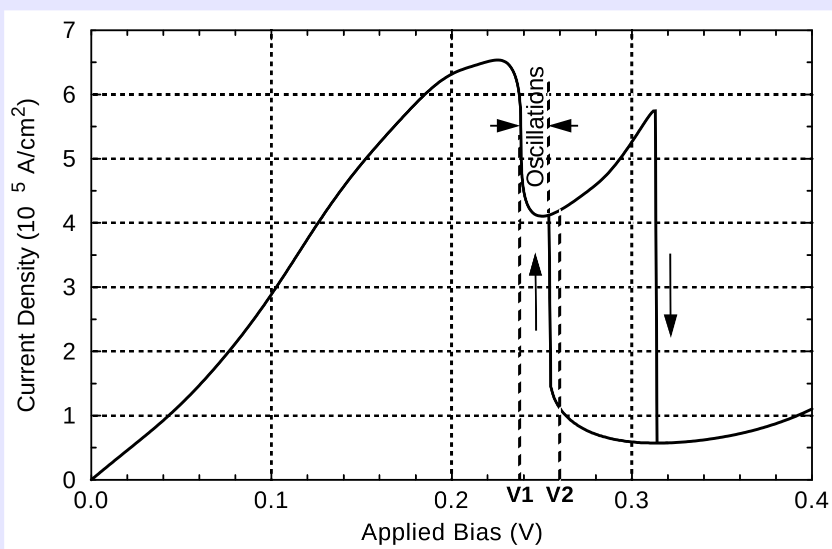
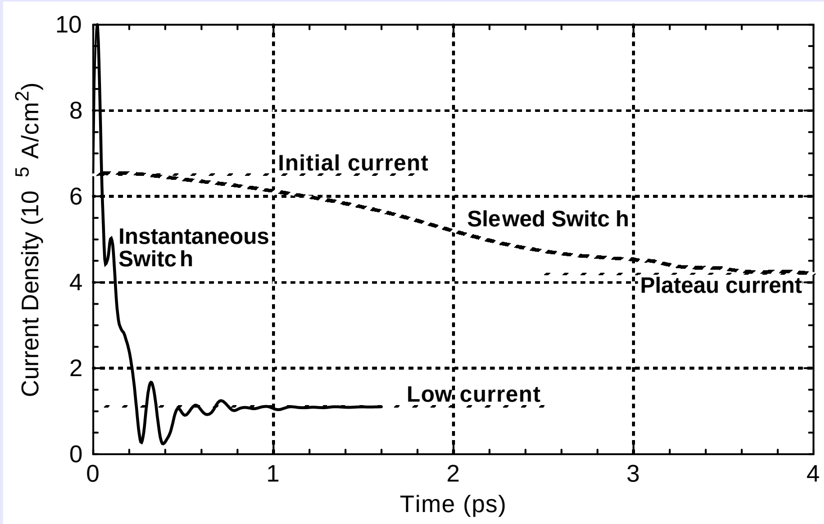
Quantum Device Simulation: Resonant Tunneling



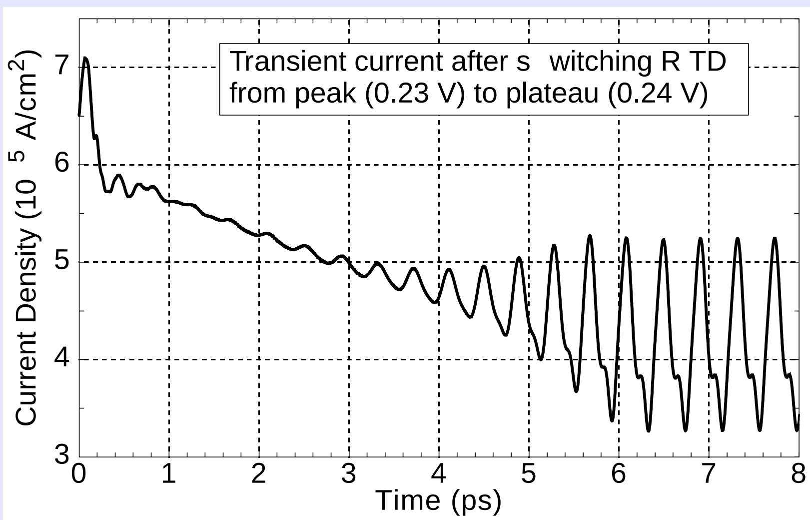
Quantum Device Simulation: Intrinsic Hysteresis and Bistability



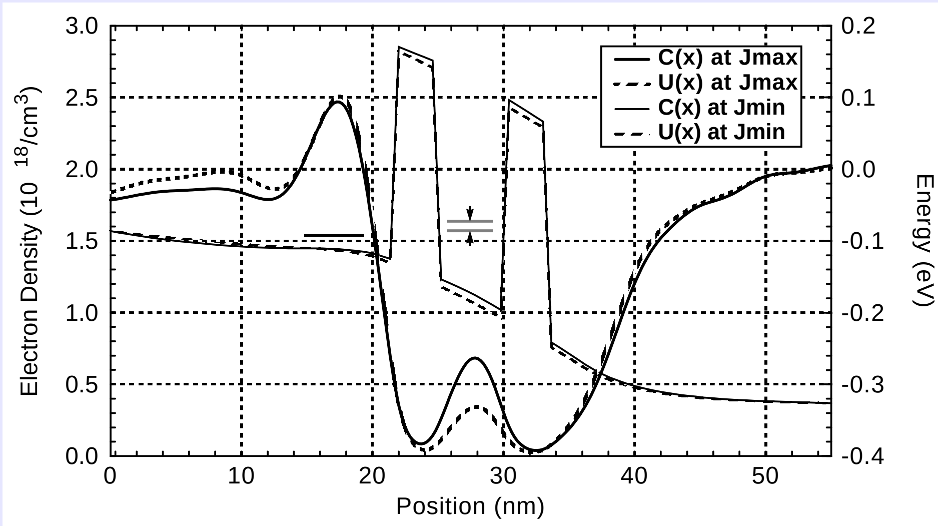
Quantum Device Simulation: Tristable Operation



Quantum Device Simulation: High Frequency Self-Oscillations



Quantum Device Simulation: Scattering into "Hidden" Quantum States



Quantum Corrections: Motivation

Conventional electronic device models tuned for efficiency and accuracy

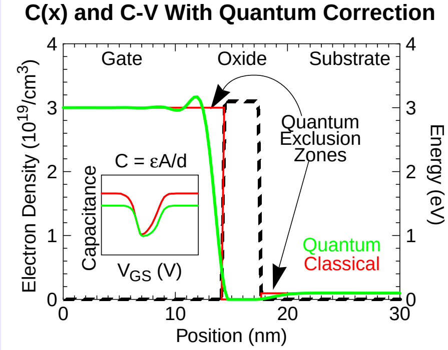
Accuracy degrades with each device generation due to quantum effects

Rather than abandoning existing software, add quantum corrections

The Wigner function formulation of quantum mechanics can be used to derive quantum corrections to main classical transport models:

- drift-diffusion
- hydrodynamic
- Boltzmann transport equation

MOSFET with 3.3 nm Gate-Oxide:
C(x) and C-V With Quantum Correction



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Quantum Corrections: Drift-Diffusion Model

Density-Gradient Model [Ancona, *PRB* **39**(13), 9536]:

$$\begin{aligned}
\nabla \cdot (\varepsilon \nabla \psi) &= -q(p - n + N_D^+ - N_A^-) \\
\frac{\partial n}{\partial t} &= \nabla \cdot [D_n \nabla n - n\mu_n \nabla(\psi + \psi_{qn})] \\
\frac{\partial p}{\partial t} &= \nabla \cdot [D_p \nabla p + p\mu_p \nabla(\psi + \psi_{qp})]
\end{aligned}$$

Quantum potentials:

$$\psi_{qn} \equiv 2b_n\left(\frac{\nabla^2\sqrt{n}}{\sqrt{n}}\right),\ \psi_{qp} \equiv -2b_p\left(\frac{\nabla^2\sqrt{p}}{\sqrt{p}}\right),\ b_{n,\,p} \equiv \frac{\hbar^2}{12 m^*_{n,\,p} q}$$

Implementation Challenges:

- 1-D, 2-D, 3-D capability
- Grid-independent
- Extensible (e.g., position-, temperature-, density-dependent $b_{n,\,p}$)

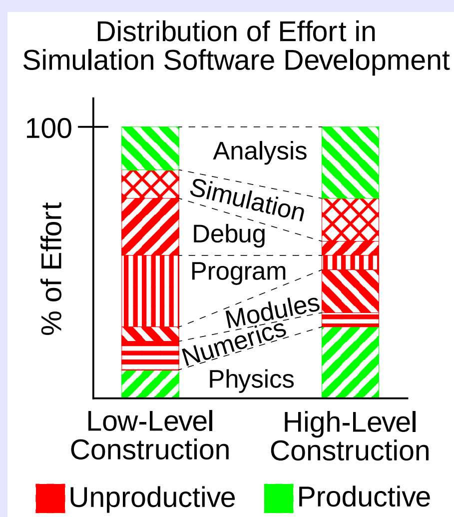
Quantum Corrections: Approach

Unproductive time between defining physical model and analyzing simulation results should be minimized. This time includes:

- Deriving numerical model
- Incorporating third-party code to reduce programming task
- Programming (writing the software)
- Debugging the software
- Waiting for simulation results

Conclusion: Simulation software should be built at the highest possible level.

In theory, all components of unproductive time except simulation can be virtually eliminated.

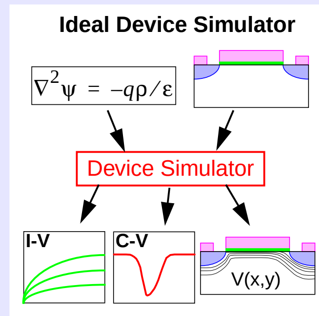


Quantum Corrections: Software Tools

Many classical models and quantum corrections need to be rapidly investigated

Ideal electronic device simulator:

- Model description as system of PDEs
- Simple specification of device structure, material parameters, device tests
- Automatic selection of numerical algorithms
- High-quality graphical output



Software tools under consideration/evaluation:

- PROPHET (General PDE solver)
- PDE Solver under development in NAS Process Modeling Group
- NAS Parallel equation solver codes (linear and non-linear systems)
- NAS 3-D Poisson Solver, 3-D Dynamic gridding codes
- Various computational fluid dynamics (CFD) codes